INFLUENCE OF BEAM DIVERGENCE AND CRYSTAL MOSAIC STRUCTURE UPON PARAMETRIC X-RAY RADIATION CHARACTERISTICS

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Abstract

Based on kinematic model of parametric X-ray radiation (PXR), an approach for calculation of PXR characteristics (spectrum, intensity, polarization and yield) has been developed. The approach allows to take into account the beam divergence, mosaicity, aperture sizes, influence of K-edge, etc. using a uniform technique.

1. The existing theoretical models [1-3] describe the process of parametric X-ray radiation (PXR) for the monodirected charged particles beam interacting with sufficiently thin ideal crystals whose multiple scattering can be neglected. The real conditions of an experiment, however, are far from being ideal.

To provide a quantitative comparison of the theoretical and experimental data we have to correctly take into account such phenomena as beam divergence, mosaicity, detector's finite aperture, effects of the K-edge absorption and some other factors.

The authors of [4] developed a phenomenological approach making it possible to approximately account for the effects of multiple scattering of particles in the target upon photon angular distribution and PXR spectrum. They assumed that multiple scattering leads to effective broadening of angular distribution of virtual photons connected with incidence particle. This approach made it possible to describe the experimental results obtained for thin perfect crystals. However, in the experiments [5-7] there was noted a significant discrepancy between the data by the proposed model and those of the experiment. The authors of [5] observed that angular distribution of PXR became narrower with decreasing electron energy. Experimental results in [6,7] show that the widths of orientational dependences (OD) of PXR yield are essentially less than the calculated values for the thick crystal target used. The authors of work [6] proposed an approach where the processes of PXR emission and multiple scattering are independent (incoherent model). This approach gives results close to the experiment and may be used for corrected account of multiple scattering.

In [8] it was shown theoretically that mosaicity of crystal target has no effect on the total PXR intensity. Recently in [9] studied experimentally were mosaic structure effects on the PXR yield and spectral characteristics. The results obtained for higher orders of PXR show disagreement with the model [4]. The authors of [10] developed a method for the account of mosaicity based on convolution of PXR angular distribution with effective distribution including multiple scattering and mosaicity in the same manner. The effect of these factors must be different. The present work offers an approach providing a uniform technique, within the kinematic model, to calculate the PXR characteristics (spectrum, polarization, angular spread, photon yield into a finite aperture for any experimental environment, photon yield into an open cone, brightness, i.e. the PXR intensity per a solid angle unit) taking

into account all the factors enumerated earlier.

2. As an assumed expression we chose the formula derived in [11] as the most clear:

$$\frac{dN}{dZ} = \frac{\sum_\alpha \alpha\omega^3 |\chi_{\vec{g}}|^2 d\Omega}{2\pi\varepsilon_0^{3/2}\beta(1-\sqrt{\varepsilon_0}\vec{\beta}\vec{n})}\Big[\frac{(\sqrt{\varepsilon_0}\omega\vec{\beta}-\vec{g})\vec{e}_{\vec{k}\alpha}}{(\vec{k}_\perp+\vec{g}_\perp)^2+\frac{\omega^2}{\beta^2}\{\gamma^{-2}+\beta^2(1-\epsilon_0)\}}\Big]^2. \quad (1)$$

Here and later in the text use is made of the system of units $\hbar = m_e = c = 1$. In Eq.(1) $\varepsilon_0 = 1 - \omega_p^2/\omega^2$, ω_p is the plasma frequency, $\vec{\beta} = \beta\vec{n}_0$ is the initial particle (electron) velocity, $\vec{n}_0$, $\vec{n}$ are the unit vectors in the direction of the initial electron and the PXR photon (with the energy ω and momentum $\vec{k}$), $\vec{g}$ is the reciprocal lattice vector, $\vec{e}_{\vec{k}\alpha}$ are the polarization unit vectors, $\perp$ is the index denoting the projection of vectors into the plane perpendicular to $\vec{n}$. By $|\chi_{\vec{g}}|$ we denote here the following value:

$$|\chi_{\vec{g}}|^2 = |S(\vec{g})|^2 \exp(-2W)\Big[-\frac{\omega_p^2}{\omega^2}\frac{F(\vec{g})}{z}\Big]^2. \quad (2)$$

In Eq.(2), $|S(\vec{g})|^2$ is the structure factor, $\exp(-2W)$ in the Debye-Waller factor, $F(\vec{g})$ is the Fourier component of the spatial distribution of electrons in the crystal atom, with $F(0) = z$, where z is the total number of electrons in the atom.

For the sake of convenience let us introduce the following coordinate systems :

1) The main system (x, y, z) where the z-axis is directed along the electron momentum, i.e. $\vec{n}_0 = \{0, 0, 1\}$. The y axis is normal to the diffraction plane, i.e. the vectors $\vec{g}, \vec{n}, \vec{n}_0$ are placed on the (xz) plane.

2) The coordinate system indexed (g) is related to the $\vec{g}$ vector that is directed along z_g. The g system is rotated with respect to the main system to an angle of $-(\frac{\pi}{2} - \theta_{\rm B})$ around the y-axis. Here $\theta_{\rm B}$ is used to denote the crystal alignment angle (Bragg angle).

3) The (d) index denotes the detector's system related to the emitted photon, which is rotated with respect to the main system to an angle of $\theta_d = 2\theta_{\rm B}$ around the y -axis. The photon momentum in this system has the following components:

$$\vec{k} = \omega\vec{n} = \omega\{n_{xd}, n_{yd}, n_{zd}\} = \omega\{\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta\}$$

The polar angle is measured from the Bragg direction coinciding with z_d, and the azimuthal angle - from the diffraction plane $(x_d z_d)$. In the small angle approximation

$$\vec{n} = \{\theta\cos\varphi, \theta\sin\varphi, 1 - \frac{\theta^2}{2}\} = \{\theta_x, \theta_y, 1 - \frac{\theta_x^2 + \theta_y^2}{2}\}$$

Here and later θ_x, θ_y point the component angles of the PXR photon emission in the d system.

For the sake of illustration we write the transformation of the $\vec{g}$ and $\vec{n}$ vectors during transit into the main system:

$$\begin{cases} g_x = g_{xg}\sin\theta_{\mathrm{B}} - \mathrm{g_{zg}}\cos\theta_{\mathrm{B}} \\ \qquad g_y = g_{yg} \\ g_z = g_{zg}\sin\theta_{\mathrm{B}} + \mathrm{g_{xg}}\cos\theta_{\mathrm{B}} \end{cases} \qquad \begin{cases} n_x = n_{xd}\cos\theta_d + n_{zd}\sin\theta_d \\ \qquad n_y = n_{yd} \\ n_z = n_{zd}\cos\theta_d - n_{xd}\sin\theta_d \end{cases}$$

For an ideal crystal in the system selected we have $g_{xg} = g_{yg} = 0$, $g_{zg} = g$. Write down the expression (1) making evident the dependence of the photon emission angles (taking into account that $\omega_p^2 << \omega^2$):

$$\frac{dN}{dZ} = \frac{\alpha\omega|\chi_{\vec{g}}|^2}{2\pi(1 - \frac{3}{2}\frac{\omega_p^2}{\omega^2})(1 - \frac{1}{2\gamma^2})[1 - (1 - \frac{\omega_p^2}{2\omega^2})(1 - \frac{1}{2\gamma^2})\cos\theta_d]}\Lambda d\Omega =$$

$$= \frac{\alpha\omega|\chi_{\vec{g}}|^2}{2\pi(1 - \cos\theta_d)}\Lambda d\Omega. \qquad (1a)$$

where the angular photon pattern is described by the following distribution:

$$\Lambda = \frac{\sum_\alpha |((1 - \frac{1}{2\gamma^2})\vec{n}_0 - \frac{\vec{g}}{\omega})\vec{e}_{\vec{k}\alpha}|^2}{\left[(\frac{\vec{k}_\perp}{\omega} + \frac{\vec{g}_\perp}{\omega})^2 + \gamma^{-2} + \frac{\omega_p^2}{\omega^2}\right]^2}. \qquad (1b)$$

The expressions (1a) and (1b) were derived using the approximation $\gamma >> 1$. In Eqs. (1a), (1b) and later by ω we denote the PXR photon energy that is defined using the conservation laws and depends on the crystal alignment and photon emission angles in the following manner [11]:

$$\omega = \frac{\vec{g}\vec{n}_0}{\frac{1}{\beta} - \sqrt{\epsilon_0}\vec{n}\vec{n}_0} \qquad (3)$$

Introduce the unit polarization vector: $\vec{e}_{\vec{k}1} = \dfrac{[\vec{n}, \vec{n}_0]}{|[\vec{n}, \vec{n}_0]|}$, $\vec{e}_{\vec{k}2} = [\vec{e}_{\vec{k}1}, \vec{n}]$. Now in the detector's system we obtain the following expressions for $\vec{e}_{\vec{k}\alpha}$:

$$\vec{e}_{\vec{k}1} = \left\{ \frac{n_{yd}}{\sin\theta_d\sqrt{1+2\cot\theta_d n_{xd}}}, -\frac{n_{xd}\cos\theta_d + \sin\theta_d}{\sin\theta_d\sqrt{1+2\cot\theta_d n_{xd}}}, 0 \right\}$$

$$\vec{e}_{\vec{k}2} = \left\{ -\frac{n_{xd}\cos 2\theta_d + \sin\theta_d\cos\theta_d}{\sin\theta_d\sqrt{1+2\cot\theta_d n_{xd}}}, -\frac{n_{yd}\cos\theta_d}{\sin\theta_d\sqrt{1+2\cot\theta_d n_{xd}}}, \right.$$
$$\left. \frac{2n_{xd}\sin\theta_d\cos\theta_d + \sin^2\theta_d}{\sin\theta_d\sqrt{1+2\cot\theta_d n_{xd}}} \right\}$$

From the above follows: $\vec{n}_0\vec{e}_{\vec{k}1} = 0$, $\vec{n}_0\vec{e}_{\vec{k}2} = \sin\theta_d\sqrt{1+2\cot\theta_d n_{xd}}$,

$$\vec{g}\vec{e}_{\vec{k}1} = -\frac{g n_{yd}\cos\theta_{\rm B}}{\sin\theta_d\sqrt{1+2\cot\theta_d n_{xd}}}, \tag{4}$$

$$\vec{g}\vec{e}_{\vec{k}2} = \frac{g[\sin\theta_d\cos(\theta_d-\theta_{\rm B}) + {\rm n_{xd}}\cos(2\theta_{\rm d}-\theta_{\rm B})]}{\sin\theta_d\sqrt{1+2\cot\theta_d n_{xd}}}$$

Substituting (4) into (1b) and summing with respect to polarization we can obtain the numerator in the following form

$$\sum_\alpha \left| \Big((1-\frac{1}{2\gamma^2})\vec{n}_0 - \frac{\vec{g}}{\omega} \Big)\vec{e}_{\vec{k}\alpha} \right|^2 = \frac{1}{\sin^2\theta_d(1+2\cot\theta_d n_{xd})} \times$$
$$\times \left\{ \frac{g^2}{\omega^2}n_{yd}^2\cos^2\theta_{\rm B} + \Big[(1-\frac{1}{2\gamma^2})\sin^2\theta_{\rm d}(1+2\cot\theta_{\rm d}{\rm n_{xd}}), \right.$$
$$\left. -\frac{g}{\omega}(\sin^2\theta_d\cos(\theta_d-\theta_{\rm B}) + {\rm n_{xd}}\cos(2\theta_{\rm D}-\theta_{\rm B}) \Big) \Big]^2 \right\}. \tag{5}$$

From Eq.(3) we can get the relation:

$$\frac{g}{\omega} = \frac{1}{\sin\theta_B}\Big[1 - \cos\theta_d + n_{xd}\sin\theta_d +$$
$$+ \cos\theta_d\frac{n_{xd}^2 + n_{yd}^2}{2} + \frac{1}{2\gamma^2} + \frac{\omega_p^2}{2\omega^2}\cos\theta_d \Big]. \tag{3a}$$

For Bragg direction ($n_{xd} = n_{yd} = 0$) from Eq.(3) we can, using the equity $1 - \cos\theta_d = 1 - \cos 2\theta_\mathrm{B} = 2\sin^2\theta_\mathrm{B}$, obtain:

$$\omega_\mathrm{B} = \frac{\mathrm{g}\sin\theta_\mathrm{B}}{1 - \cos\theta_\mathrm{d} + \dfrac{1}{2\gamma^2} + \dfrac{\omega_\mathrm{p}^2}{\omega^2}\cos\theta_\mathrm{d}} = \frac{\mathrm{g}}{2\sin\theta_\mathrm{B}}\left(1 - \frac{\gamma^{-2} + \dfrac{\omega_\mathrm{p}^2}{\omega^2}\cos\theta_\mathrm{d}}{4\sin^2\theta_\mathrm{B}}\right) \qquad (3b)$$

For the geometry corresponding to large alignment angles ($\theta_\mathrm{B} \;>> \gamma^{-1}$, ω_p/ω), following Eq.(3b) we have: $\omega_\mathrm{B} = \frac{\mathrm{g}}{2\mathrm{sin}\theta_\mathrm{B}}$, which agrees with the Bragg law for real X-ray photon diffraction. For small deviation from the Bragg direction ($n_{xd},\ n_{yd} << 1$) we can obtain an expression simpler than a somewhat awkward Eq.5. Upon substituting Eq.(3a) into Eq.(5) leaving in the expansion the terms not higher that n_{xd}^2, n_{yd}^2, we obtain:

$$\sum_\alpha \left|\left((1 - \frac{1}{2\gamma^2})\vec{n}_0 - \frac{\vec{g}}{\omega}\right)\vec{e}_{\vec{k}\alpha}\right|^2 = n_{xd}\gamma^{-2}\sin\theta_d\cos\theta_d + n_{xd}^2\cos^2 2\theta_\mathrm{B} +$$

$$+ n_{yd}^2 = \theta_x\gamma^{-2}\sin\theta_d\cos\theta_d + \theta_x^2\cos^2 2\theta_\mathrm{B} + \theta_y^2 \qquad (6)$$

The denomination in Eq.(1) is calculated in the main system where

$$\frac{\vec{k}_\perp}{\omega} = \left\{n_{xd}\cos\theta_d - \sqrt{1 - n_{xd}^2 - n_{yd}^2}\sin\theta_d,\ \ n_{yd},\ \ 0\right\}$$

$$\frac{\vec{g}_\perp}{\omega} = \left\{-\frac{g}{\omega}\cos\theta_\mathrm{B},\ 0,\ 0\right\}$$

Upon calculating in a similar approximation we get:

$$\left[\left(\frac{\vec{k}_\perp}{\omega} + \frac{\vec{g}_\perp}{\omega}\right)^2 + \frac{1}{\beta^2\gamma^2} + 1 - \epsilon_0\right]^2 = \left[n_{xd}^2 + n_{yd}^2 + \gamma^{-2} + \frac{\omega_p^2}{\omega^2}\right]^2 =$$

$$= (\theta_x^2 + \theta_y^2 + \theta_{ph}^2)^2 \qquad (7)$$

Here θ_{ph} is used to indicate the angle $\theta_{ph} = \sqrt{\gamma^{-2} + \omega_p^2/\omega^2}$. Thus, the angular distribution of the PXR response with respect to the Bragg direction is described by the following expression:

$$\Lambda(\theta_x, \theta_y) = \frac{\theta_x\gamma^{-2}\sin\theta_d\cos\theta_d + \theta_x^2\cos^2 2\theta_\mathrm{B} + \theta_y^2}{\left[\theta_x^2 + \theta_y^2 + \gamma^{-2} + \dfrac{\omega_p^2}{\omega^2}\right]^2} \qquad (8)$$

For an ultrarelativistic case, when $\theta_x \sim \gamma^{-2}$, the first summand in the numerator may be neglected. The expression thus obtained appears, as to it is be expected, to agree with a well-known distribution [4]. In the expression (8), however, the summand linear with respect to θ_x gives an asymmetric contribution into the PXR angular distribution in the horizontal plane. This contribution increases with decreasing electron energy. It is this summand which determines the asymmetry of the PXR orientation dependence measured in the experiment [12] for the electron energy $E_e = 25$ MeV. Using Eqs.(1a) and (8) we can obtain the PXR intensities into open cone around Bragg direction. Replacing n_{xd}, n_{yd} and n_{zd} by their values in the spherical coordinate system we get the following:

$$\Lambda = \frac{\gamma^{-2}\sin\theta\cos\varphi\sin\theta_d\cos\theta_d + \sin^2\theta(\cos^2 2\theta_{\rm B}\cos^2\varphi + \sin^2\varphi)}{\left[\sin^2\theta + \gamma^{-2} + \dfrac{\omega_p^2}{\omega^2}\right]^2}$$

which is readily integrated,

$$\Upsilon = \int\limits_0^{\pi} \sin\theta d\theta \int\limits_0^{2\pi} d\varphi \Lambda(\theta,\varphi) = \pi(1+\cos^2 2\theta_{\rm B})\left[\ln\frac{2}{\theta_{ph}^2} - 1\right]$$

Upon integrating Eq.(1a) with respect to the crystal thickness L (taking into account the absorption) we obtain the well-known expression [3]:

$$N_0 \approx \frac{\alpha\omega_{\rm B}(1+\cos^2 2\theta_{\rm B})|\chi_{\vec{g}}|^2}{2(1-\cos 2\theta_{\rm B})}\Big(\ln\frac{2}{\theta_{ph}^2} - 1\Big)L_a\Big(1-\exp\,(-\frac{L}{L_a})\Big) \qquad (9)$$

Where L_a is the absorption length of photon with the energy $\omega_{\rm B}$.

3. In order to make account of real experimental conditions (beam divergence, mosaicity, finite aperture of the detector, etc.) we propose a simple algorithm. Let the beam divergence be described by the distribution $F_e(\Delta_x, \Delta_y)$ and the mosaic structure by $F_m(\alpha_x, \alpha_y)$. Using the approximations $\Delta_{x,y} << 1$, $\alpha_{x,y} << 1$, which are almost always true, we may assume the PXR angular distribution to be invariable (i.e. $\omega_{\rm B}$, $\theta_{\rm ph} = $ const). Changes occur only in the Bragg direction which is used to determine the angles θ_x, θ_y in Eq.(8). It can be demonstrated that for the electrons with the incidence angles Δ_x, Δ_y (determined with respect to the mean direction $<\vec{n}_0>$) shift of the Bragg direction in the d - system is found using the following:

$$n_{xd}^{\rm B} = -\cos\Delta_y\sin\Delta_x \approx -\Delta_x$$

$$n_{yd}^{\mathrm{B}} = \sin\Delta_y \approx \Delta_y \tag{10a}$$

$$\Delta_{zd}^{\mathrm{B}} = \cos\Delta_y \cos\Delta_x \approx 1 - \frac{\Delta_x^2 + \Delta_y^2}{2}$$

The mosaic distribution function $F_m(\alpha_x, \alpha_y)$ is defined with respect to the mean direction of $< \vec{g} >$, i.e. in the g-system. The Bragg direction for an element of mosaic structure corresponding to the reciprocal lattice vector $\vec{g}_g = g\{\alpha_x, \alpha_y, 1 - \dfrac{\alpha_x^2 + \alpha_y^2}{2}\}$ will be determined as

$$n_{xd}^{\mathrm{B}} = -\sin 2\theta_{\mathrm{B}} \sin^2\alpha_{\mathrm{y}} + \sin 2\alpha_{\mathrm{x}} \cos^2\alpha_{\mathrm{y}} \approx 2\alpha_{\mathrm{x}}$$

$$n_{yd}^{\mathrm{B}} = -\sin 2\alpha_y \sin(\theta_{\mathrm{B}} + \alpha_{\mathrm{x}}) \approx -2\alpha_{\mathrm{y}} \sin\theta_{\mathrm{B}} \tag{10b}$$

$$n_{zd}^{\mathrm{B}} = \cos 2\theta_{\mathrm{B}} \sin^2\alpha_{\mathrm{y}} + \cos^2\alpha_{\mathrm{y}} \cos 2\alpha_{\mathrm{x}} \approx 1 - 2\alpha_{\mathrm{x}}^2 - 2\alpha_{\mathrm{y}}^2 \sin^2\theta_{\mathrm{B}}$$

Thus, for PXR generation by a diverging electron beam, the photon angular spread with respect to the mean Bragg direction can be written using the convolution:

$$\Lambda_e(\theta_x, \theta_y) = \int d\Delta_x d\Delta_y F_e(\Delta_x, \Delta_y) \Lambda(\theta_x + \Delta_x, \theta_y - \Delta_y) \tag{11}$$

If, alongside with the diverging beam, we have a mosaic crystal then we get an angular spread of the form:

$$\begin{aligned} \Lambda_{e,m}(\theta_x, \theta_y) &= \int d\alpha_x d\alpha_y F_m(\alpha_x, \alpha_y) \Lambda_e(\theta_x - 2\alpha_x, \theta_y + 2\alpha_y \sin\theta_{\mathrm{B}}) = \\ &= \int d\alpha_x d\alpha_y F_m(\alpha_x, \alpha_y) \int d\Delta_x d\Delta_y F_e(\Delta_x, \Delta_y) \times \\ &\quad \times \Lambda(\theta_x + \Delta_x - 2\alpha_x, \theta_y - \Delta_y + 2\alpha_y \sin\theta_{\mathrm{B}}) \end{aligned} \tag{12}$$

In order to provide the PXR yield into a finite detector's aperture Eq.(12) should be integrated with respect to the aperture $\Delta\Omega$:

$$N_{\mathrm{PXR}} = \mathrm{const} \int_{\Delta\Omega} \mathrm{d}\theta_{\mathrm{x}} \mathrm{d}\theta_{\mathrm{y}} \Lambda_{\mathrm{e,m}}(\theta_{\mathrm{x}}, \theta_{\mathrm{y}})$$

This expression could be simplified by introducing the variables $\xi_x = \Delta_x - 2\alpha_x$, $\xi_y = -\Delta_y + 2\alpha_y \sin\theta_B$. Then the internal integral in Eq.(12) will have the form:

$$-\int d\xi_x d\xi_y F_e(\xi_x + 2\alpha_x, -\xi_y + 2\alpha_y \sin\theta_{\mathrm{B}}) \Lambda(\theta_{\mathrm{x}} + \xi_{\mathrm{x}}, \theta_{\mathrm{y}} + \xi_{\mathrm{y}})$$

and the integral is transformed into:

$$\Lambda_{e,m}(\theta_x,\theta_y) = -\int\int d\alpha_x d\alpha_y F_m(\alpha_x,\alpha_y) d\xi_x d\xi_y \times$$

$$\times F_e(\xi_x + 2\alpha_x, -\xi_y + 2\alpha_y \sin\theta_{\mathrm{B}})\Lambda(\theta_{\mathrm{x}} + \xi_{\mathrm{x}}, \theta_{\mathrm{y}} + \xi_{\mathrm{y}})$$

If the effective angular distribution function is introduced, then

$$F_{eff}(\xi_x,\xi_y) = -\int d\alpha_x d\alpha_y F_m(\alpha_x,\alpha_y) F_e(\xi_x + 2\alpha_x, -\xi_y + 2\alpha_y \sin\theta_{\mathrm{B}}), \quad (13)$$

which in a number of cases can be analytically calculated (e.g. when F_m and F_e are Gaussian distributions), then instead of Eq.(12) we get:

$$\Lambda_{e,m}(\theta_x,\ \theta_y) = \int d\xi_x d\xi_y F_{eff}(\xi_x,\xi_y)\Lambda(\theta_x + \xi_x, \theta_y + \xi_y) \quad (14)$$

For illustrative purposes let us calculate the effective angular distribution $F_{eff}(\xi_x, \xi_y)$ when $F_m(\alpha_x,\ \alpha_y)$ and $F_e(\Delta_x, \Delta_y)$ are approximated by the Gaussians :

$$F_m(\alpha_x,\alpha_y) = \mathrm{C}_1\exp\{-\frac{\alpha_{\mathrm{x}}^2}{2\sigma_{\mathrm{m}}^2}\}\exp\{-\frac{\alpha_{\mathrm{y}}^2}{2\sigma_{\mathrm{m}}^2}\},$$

$$F_e(\Delta_x,\Delta_y) = \mathrm{C}_2\exp\{-\frac{\Delta_{\mathrm{x}}^2}{2\sigma_{\mathrm{x}}^2}\}\exp\{-\frac{\Delta_{\mathrm{y}}^2}{2\sigma_{\mathrm{y}}^2}\}$$

The latter approximation can describe the electron beam angular divergence with different dispersion along x and y.In this case the effective angular distribution, Eq.(13), is readily calculated:

$$F_{eff}(\xi_x,\xi_y) = \mathrm{C}_3 \exp\{-\frac{\xi_{\mathrm{x}}^2}{2\sigma_{\mathrm{x}}^2(1+4\sigma_{\mathrm{m}}^2/\sigma_{\mathrm{x}}^2)}\}\exp\{-\frac{\xi_{\mathrm{y}}^2}{2\sigma_{\mathrm{y}}^2(1+4\sin^2\theta_{\mathrm{B}}\sigma_{\mathrm{m}}^2/\sigma_{\mathrm{y}}^2)}\}$$

This results in broadened Gaussians with the dispersions $\sqrt{\sigma_x^2 + 4\sigma_m^2}$ and $\sqrt{\sigma_y^2 + 4\sigma_m^2 \sin^2\theta_{\mathrm{B}}}$.

The effect of the mosaic structure along the x-axis is four times that of the divergence.

4. Let us consider in a greater detail the effects of divergence and mosaic structure on PXR angular distribution. For the sake of convenience we consider one - dimensional distribution along the y axis.

a) Let the beam divergence be described by the following distribution:

$$F_e(\Delta_x,\Delta_y)=\frac{1}{2\pi\sigma_e^2}\exp(-\frac{\Delta_x^2+\Delta_y^2}{2\sigma_e^2})=F_e(\Delta_x)F_e(\Delta_y),$$

with $\int d\Delta_x F_e(\Delta_x)=\int d\Delta_y F_e(\Delta_y)=1$

Then the resulting angular distribution of PXR in vertical direction has the form:

$$\widetilde{\Lambda}(\theta_y)=\int d\theta_x\int d\Delta_x d\Delta_y F_e(\Delta_x)F_e(\Delta_y)\Lambda(\theta_x+\Delta_x,\theta_y-\Delta_y)$$

If we change the sequence of integration in this expression we may analy tically calculate the integral

$$\int d\theta_x\Lambda(\theta_x+\Delta_x,\theta_y-\Delta_y)\simeq\int d\theta_x\Lambda(\theta_x,\theta_y-\Delta_y),$$

since the integration limits can approach $\pm\infty$. As a result we obtain

$$\Lambda(\theta_y-\Delta_y)=\int d\theta_x\Lambda(\theta_x,\theta_y-\Delta_y)=$$

$$=\frac{\pi}{2}\frac{\theta_{ph}^2\cos^2\theta_{\rm B}+(\theta_{\rm y}-\Delta_{\rm y})^2(1+\cos^2 2\theta_{\rm B})}{[\theta_{ph}^2+(\theta_y-\Delta_y)^2]^{\frac{3}{2}}} \tag{15}$$

Now integration with respect to $d\Delta_x$ becomes trivial. Thus

$$\widetilde{\Lambda}(\theta_y)=\int d\Delta_y F_e(\Delta_y)\Lambda(\theta_y-\Delta_y) \tag{16}$$

Consider the case with $\theta_{\rm B}=\pi/4$. Shown in Fig.1 curve 1 is the distribution of Eq.(8) for ideal case ($\Delta_y=0$) versus a dimensionless variable $y=\dfrac{\theta_y}{\theta_{ph}}$. One may see a double-lobe distribution with maxima at $y_0=\pm\sqrt{2}$. As follows from the expressions obtained, the effects of beam divergence (and, therefore those, of multiple scattering) are reduced to the broadening maxima, the decrease of the dip of minimum, however, producing small effect on the position of the maxima.

In Fig.1 curve 2 shows the convolution of the distribution (16) with the Gaussian $F_e(\Delta_y)$ for the dispersion $\sigma_e=\theta_{ph}$.One may notice a slight shift

of the maxima towards the region of large values. Nevertheless, the derived value of y_0 is by far lower than it follows from a well known model [4]:

$$y_0 < \sqrt{\theta_{ph}^2 + \sigma_e^2}/\theta_{ph}.$$

It should be noted that the value of distribution contrast $\widetilde{\Lambda}(\theta_y)$ (the ratio of the intensity at its maximum and minimum) can be used to define the angular distribution of the initial beam.

b) Mosaic structure effects could be considered in a similar manner. Convolution of the Gaussian with the dispersion σ_m^2 with the expression (15), was shown in Fig.2, where

$$\theta_y' = \theta_y + 2\alpha_y \sin\theta_{\rm B}$$

Very roughly one can estimate the value of dispersion σ_m^2 where in the distribution the two maxima are smoothed and a single peak appears at $\theta_y = 0$; $1.18\sigma_m > \sqrt{2}\theta_{ph}\sin\theta_{\rm B}$, or $\sigma_m > 1.25\theta_{ph}\sin\theta_{\rm B}$.

Drawn in Fig.2 are the results of convolution of the exact distribution for different dispersions $\sigma_m = \theta_{ph}$ and $2\theta_{ph}$. As follows from the figure the double - lobe distribution of PXR virtually disappears.

5. It follows from Eq.(3) that the shape and width of the PXR spectral line are defined by the electron beam divergence, crystal mosaic structure and the collimator aperture. In order to obtain the shape of spectral line we have to introduce the variable $\theta_x = \theta_x(\omega)$ and then integrate the expression with respect to the remaining variable θ_y. To make a simultaneous account of the effects of divergence and mosaic structure let us obtain the relation between the PXR photon energy and the angles used in the problem. Substituting values of the vectors $\vec{g}, \vec{n}$, and $\vec{n}_0$ in the main system into Eq.(3) we get the sought - for dependence for the energy of PXR photons emitting in the direction given n_{xd}, n_{yd} in a mosaic crystal for the electrons of a diverging beam:

$$\omega = g\{\alpha_x\Delta_x \sin\theta_{\rm B} - \Delta_{\rm x}\cos\theta_{\rm B} + \alpha_{\rm y}\Delta_{\rm y} + \alpha_{\rm x}\cos\theta_{\rm B} + \sin\theta_{\rm B}\times$$

$$\times(1 - \frac{\alpha_x^2 + \alpha_y^2 + \Delta_x^2 + \Delta_y^2}{2})\}/\Big[1 - \Delta_x(n_{xd}\cos\theta_d + \sin\theta_d) -$$

$$-\Delta_y n_{yd} + n_{xd}\sin\theta_d - \cos\theta_d + \cos\theta_d \times \frac{1}{2}(\Delta_x^2 + \Delta_y^2 + n_{xd}^2 + n_{yd}^2)\Big]$$

In the above equation we left the second-order terms. In a more rough approximation, leaving the terms up to the first order, we have:

$$\omega = \frac{g \sin\theta_{\mathrm{B}}\{1 + (\alpha_{\mathrm{x}} - \Delta_{\mathrm{x}})\cot\theta_{\mathrm{B}}\}}{(1-\cos\theta_d)\{1 + \frac{\sin\theta_d}{1-\cos\theta_d}(n_{xd} - \Delta_x)\}}$$

For the geometry chosen $\theta_d = 2\theta_{\mathrm{B}}$, therefore

$$\omega = \omega_{\mathrm{B}}\{1 + (\alpha_{\mathrm{x}} - \Delta_{\mathrm{x}})\cot\theta_{\mathrm{B}} - (\mathrm{n}_{\mathrm{xd}} - \Delta_{\mathrm{x}})\cot\theta_{\mathrm{B}}\} =$$

$$= \omega_{\mathrm{B}}\{1 + (\alpha_{\mathrm{x}} - \mathrm{n}_{\mathrm{xd}})\cot\theta_{\mathrm{B}}\} = \omega_{\mathrm{B}}\{1 + (\alpha_{\mathrm{x}} - \theta_{\mathrm{x}})\cot\theta_{\mathrm{B}}\} \qquad (17)$$

Here one may use the new spectral variable $u = \frac{\omega - \omega_{\mathrm{B}}}{\omega_{\mathrm{B}}}\tan\theta_{\mathrm{B}} = \alpha_{\mathrm{x}} - \theta_{\mathrm{x}}$.

As is clear from the above the photon energy depends on the mosaic structure in the diffraction plane and the photon exit angle only, and is irrespective of the electron beam divergence. From Eq.(17), for $\alpha_x = 0$, we may obtain

$$\omega = \omega_{\mathrm{B}}(1 - \theta_{\mathrm{x}}\cot\theta_{\mathrm{B}}); \quad \theta_{\mathrm{x}} = -\frac{\omega - \omega_{\mathrm{B}}}{\omega_{\mathrm{B}}}\tan\theta_{\mathrm{B}}; \quad \mathrm{d}\theta_{\mathrm{x}} = -\frac{\mathrm{d}\omega}{\omega_{\mathrm{B}}}\tan\theta_{\mathrm{B}}.$$

Let us find the shape of a PXR spectral line for round aperture $\theta_x^2 + \theta_y^2 \le \theta_c^2$ aligned along the Bragg direction. For this purpose we have to integrate the distribution (8) with respect to the angle θ_y within the aperture:

$$\Lambda_c(\theta_x) = \int\limits_{-\sqrt{\theta_c^2-\theta_x^2}}^{\sqrt{\theta_c^2-\theta_x^2}} \frac{\theta_x^2\cos^2 2\theta_{\mathrm{B}} + \theta_{\mathrm{y}}^2}{(\theta_x^2 + \theta_y^2 + \theta_{ph}^2)^2} d\theta_y =$$

$$= \frac{\theta_{ph}^2 + \theta_x^2(1+\cos^2 2\theta_{\mathrm{B}})}{(\theta_{ph}^2 + \theta_x^2)^{\frac{3}{2}}}\arctan\sqrt{\frac{\theta_c^2 - \theta_x^2}{\theta_{ph}^2 + \theta_x^2}} -$$

$$-\frac{\sqrt{\theta_c^2 - \theta_x^2}(\theta_{ph}^2 + \theta_x^2\sin^2 2\theta_{\mathrm{B}})}{(\theta_{ph}^2 + \theta_c^2)(\theta_{ph}^2 + \theta_x^2)}$$

For the case where $\theta_c << \theta_{ph}$ we can write a simpler expression:

$$\Lambda_c(\theta_x) \approx \frac{\sqrt{\theta_c^2 - \theta_x^2}}{\theta_{ph}^2}\frac{\theta_c^2 - \theta_x^2\cos 2\theta_d}{\theta_{ph}^2} \qquad (18)$$

After substituting $\theta_x = -u$ into the above we get the spectral line.

Let us analyse the influence of mosaic structure on the spectral lineshape. In order to get the spectral distribution of the PXR beam in the aperture $\Delta\theta_x \sim \theta_{ph},\ \Delta\theta_y >> \theta_{ph}$ we have to use the following distribution:

$$\frac{dN}{du} = \int\limits_{\Delta\Omega} d\theta_x d\theta_y \int d\alpha_y F_m(\theta_x + u,\ \alpha_y)\times$$

$$\times\Lambda(\theta_x + 2u, \theta_y + 2\alpha_y \sin\theta_{\mathrm{B}}) \approx \int\limits_{\Delta\theta_{\mathrm{x}}} \mathrm{d}\theta_{\mathrm{x}} \mathrm{F_m}(\theta_{\mathrm{x}} + \mathrm{u})\cdot$$

$$\frac{\pi}{2}\frac{\theta_{ph}^2 + (\theta_x + 2u)^2(1 + \cos^2 2\theta_{\mathrm{B}})}{[\theta_{ph}^2 + (\theta_x + 2u)^2]^{\frac{3}{2}}}, \qquad (19)$$

To calculate the PXR spectrum emitted in the given angle θ_x (near $\omega_0 = \omega_{\mathrm{B}}(1 - \cot\theta_{\mathrm{B}}\theta_{\mathrm{x}})$), following Eq.(19) let us make a replacement, then the integrand in Eq.(19) will correspond to the spectrum sought for:

$$\frac{\partial^2 \widetilde{N}}{\partial\theta_x \partial u} = \frac{1}{\sqrt{2\pi}\sigma_m}\exp\{-\frac{(\theta_x + u)^2}{2\sigma_m^2}\}$$

$$\frac{\pi}{2}\frac{\theta_{ph}^2 + (\theta_x + 2u)^2(1 + \cos^2 2\theta_{\mathrm{B}})}{[\theta_{ph}^2 + (\theta_x + 2u)^2]^{3/2}}, \qquad (20)$$

Upon integrating (20) within aperture one may get the shape of PXR spectral line, (e.g.see Fig.3). Let $\theta_B = \dfrac{\pi}{4}$ and $\sigma_m << \theta_{ph}$. Then the energy range $|\theta_x + u| << 2\sigma << \theta_{ph}$ and,therefore,

$$\frac{\partial^2 \widetilde{N}}{\partial\theta_x \partial u} \approx \frac{1}{2\sigma_m}\sqrt{\frac{\pi}{2}}\frac{1}{\theta_{ph}}\exp\{-\frac{(\theta_x + u)^2}{2\sigma^2}\}$$

The distribution obtained has a maximum at $u_0 = -\theta_x$, i.e. at

$$\omega_0 = \omega_{\mathrm{B}}(1 + \theta_{\mathrm{x}}\cot\theta_{\mathrm{B}}).$$

Contrary to the above, at $\sigma_m >> \theta_{ph}$, position of the maximum is determined by the last term in Eq.(20):

$$u_0 = -\frac{\theta_x}{2}, \quad \omega_0 = \omega_{\mathrm{B}}(1 - \frac{\theta_{\mathrm{x}}}{2}\cot\theta_{\mathrm{B}})$$

and the spectral distribution has the form:

$$\frac{\partial^2 \widetilde{N}}{\partial\theta_x \partial u} \approx \frac{1}{2\sigma_m}\sqrt{\frac{\pi}{2}}\exp\{-\frac{\theta_x^2}{4\sigma_m^2}\}\frac{1}{\sqrt{\theta_{ph}^2 + (\theta_x + 2u)^2}}$$

In this case the energy of PXR photons is defined by the elements of mosaic structure with $\alpha_x = \theta_x + u \approx \frac{1}{2}\theta_x$ (but not by the mosaic structure with $\alpha = 0$), which results in an effective change of the angle $\widetilde{\theta_d}$:

$$\widetilde{\theta}_d = \theta_d + \theta_x$$

Summing up the above considerations we may state that the main contribution into radiation along θ_x comes from the mosaic structure elements whose direction coincides with the Bragg direction.

The approach described in previous chapter is a good approximation for the case where the PXR line is located far from the absorption edges, where the absorption length changes in a drop. In order to take the K-edge influence into account it is necessary to calculate the spectral distribution $\frac{dN}{d\omega}$ according to the method described in the previous chapter and then count the distributions of photons with the energy above and below the K-edge. These two groups of photons are absorbed in the crystal in a different manner, i.e. they have different length L_a. Using, for each of the groups, a formula similar to (9) and then finding the sum, we may obtain the photon yield near the K-edge of absorption.

6. In conclusion we would like to note the following:

a) beam divergence and crystal mosaicity effect the PXR characteristics in a different manner;

b) with increasing beam divergence (or mosaicity) the well-known two-lobe angular distribution of PXR transform into a single-lobe distribution with maximum near Bragg direction;

c) the spectral line width of PXR is defined by the collimator's aperture (or detector's) and mosaicity, but not the divergence (or multiple scattering);

d) and finally that the approach developed makes it possible to calculate (to an accuracy where the PXR kinematic theory is true) all the PXR characteristics measured without addition of any other phenomenological parameters.

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Figure Captions

Fig. 1. PXR angular distributions for $\theta_{\mathrm{B}} = \pi/4$:
1 - ideal case; 2 - convolution with beam divergence $\sigma_e = \theta_{ph}$;
3 - Feranchuk-Ivashin model for $\theta_{ph}^2 = \gamma^{-2} + \frac{\omega_p^2}{\omega^2} + \sigma^2,\ \sigma = \theta_{ph}$.

Fig. 2. PXR angular distributions for different mosaicities :
1 - $\sigma_m = 0.$; 2 - $\sigma_m = \theta_{ph}$; 3 - $\sigma_m = 2\theta_{ph}$.

Fig. 3. PXR spectral distributions for $\theta_{\mathrm{B}} = \pi/4$ and $\Delta\theta_x = \pm 0.5\theta_{ph}$
Curve 1 - $\sigma_m = 0.2\theta_{ph}$, Curve 2 - $\sigma_m = 4\theta_{ph}$.

Fig. 2

Fig. 3